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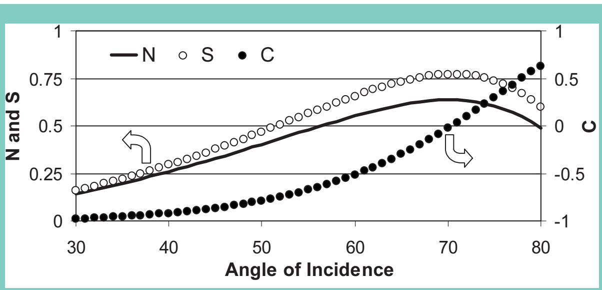

N, *C*, and *S* curves for ⟨ε⟩ = –0.44 + 6.91 *i* (Au at 300 nm)

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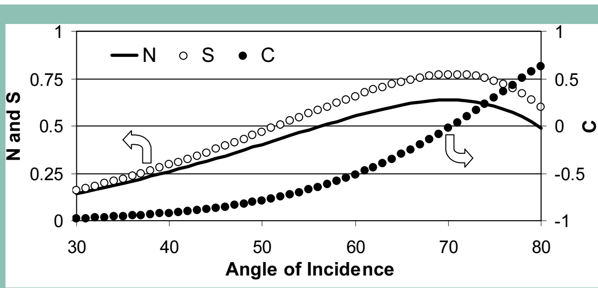
As the diversity and complexity of ellipsometric applications continue to increase, so do the requirements for ellipsometric data accuracy. In the previous ICSE-3 conference, Aspnes identified this issue, and suggested a 0.1% target for ellipsometric accuracy [1]. Unfortunately, there is no generally accepted method for characterizing or quantifying ellipsometric data accuracy. In this paper, a simple method and metric are proposed for quantifying the accuracy of an ellipsometer system.



N, *C*, and *S* curves for ⟨ε⟩ = –0.44 + 6.91 *i* (Au at 300 nm)

1 Introduction Ellipsometric accuracy is defined as the residual error between the experimentally measured and ideal values of ellipsometric data, where the experimental data are acquired/averaged over a long enough time period to reduce the random errors (noise) to negligible levels. Due to the extremely high precision and sensitivity obtainable by modern ellipsometer systems, it is essentially impossible to fabricate a reference sample in which the ideal ellipsometric values are known to a level comparable to the ellipsometric precision. For example, a procedure for creating a Si reference sample has been suggested [2], but the estimated reproducibility in the surface overlayer thickness of ±0.2 Å is more than 2 orders of magnitude larger than the achievable precision in Si oxide thickness of ≈0.001 Å [1]. The only exactly known reference for ellipsometric measurements is 'air': Ψ=45° and Δ=0° for ellipsometric measurements acquired in the 'straight-through' (S-T) configuration. While this is a useful (and necessary) test of ellipsometric accuracy, it only characterizes the accuracy of a system for ellipsometric values of Ψ near 45° and Δ near 0°. Furthermore, if S-T data is included as part of the fundamental instrument calibration procedure, S-T measurements are not an objective (and certainly not a sufficient) indication of ellipsometer system accuracy.

To determine the ellipsometric accuracy over a wider range of ellipsometric values, a simple obvious concept is exploited: for a bulk-like sample, the ellipsometrically measured pseudo-dielectric function should be essentially constant for all angles of incidence. The basic procedure is to acquire ellipsometric data vs. angle of incidence on a bulk-like sample (which measures a wide range of ellipsometric values), analyze the experimental data vs. angle with a simple substrate only optical model (fitting the pseudo-dielectric function values at each measured wavelength), and then evaluate the ellipsometric accuracy by quantifying the difference between the experimental and model generated data. With this approach, no *a priori* knowledge of the material dielectric functions is required; only the assumption of a bulk-like sample must be valid (the samples do need to be stable during the measurement time, but not necessarily over the long term). To cover a wide range of ellipsometric values and sample reflectivities, three representative reference samples are suggested for this method: a silicon wafer with native oxide, an optically thick gold film, and a polished fused silica optical flat.

We propose that a suitable metric for quantifying ellipsometric accuracy is the root mean squared (RMS) difference between the experimentally measured and ideal values of the sample Mueller matrix elements. For non- elements can be defined in terms of the traditional ellipsometric parameters as: N=cos(2Ψ), C=sin(2Ψ)cos(Δ), and S=sin(2Ψ)sin(Δ) [3].

To demonstrate the proposed method, the ellipsometric accuracy of a prototype dual rotating compensator system [4] was characterized by measuring the 3 reference samples over a 245–1700 nm spectral range, and 30–80° angle of incidence range. The RMS accuracy metric is reported for standard (isotropic) ellipsometric, depolarization, generalized ellipsometry, and Mueller matrix measurements. Limitations of this method, such as the range of ellipsometric values characterized, errors introduced by the bulk-like sample assumption, and the effects of angle of incidence errors are discussed.

2 Ellipsometric accuracy metric

Ellipsometric measurements are typically reported in terms of the parameters Ψ and Δ, which are related to the magnitude and phase of the complex reflectivity ratio as defined in equation (1) [5]. While this definition is commonly used (primarily for historical reasons), it exhibits an obvious shortcoming: the sensitivity to Δ depends on the value of Ψ. In the limiting cases, the Δ parameter is undefined if Ψ=0° or Ψ=90°. Furthermore, the Ψ and Δ parameters are not directly related to quantities experimentally measured by modern ellipsometer systems (they *are* related to the azimuth values of the optics on a classic null ellipsometer system), which implies that the precision and accuracy with which Ψ and Δ can be measured depend strongly on the type of ellipsometer system used for the measurement.

$$\tan(\Psi)e^{i\Delta} = R_p/R_s \,. \tag{1}$$

To avoid the pitfalls of the Ψ-Δ representation, some authors have reported and analyzed ellipsometric measurements from rotating polarizer or analyzer ellipsometers in terms of the measured normalized Fourier coefficients α and β [6], as opposed to calculating Ψ and Δ from α and β using the non-linear transforms shown in equation (2) [7]. However, Fourier coefficient α and β values are only applicable to rotating polarizer or analyzer ellipsometer configurations.

$$\tan(\Psi) = \sqrt{\frac{1+\alpha}{1-\alpha}}\tan(P) \;, \quad \cos(\Delta) = \beta\sqrt{\frac{1}{1-\alpha^2}} \;,$$

where P is the polarizer azimuth. (2)

An alternative representation for ellipsometric data is the N, C, and S notation described by Jellison [3]. N, C, and S are the non-zero elements of the normalized Mueller Matrix (MM) for an isotropic sample (3). For a non-depolarizing sample, they can be defined in terms of the traditional ellipsometric parameters as: N=cos2Ψ, C=sin2Ψcos Δ, and S=sin2Ψsin Δ. These quantities are bounded from −1 to +1 (as are the normalized Fourier coefficients). Furthermore, as shown in Table 1, they are linearly related to the quantities measured by the ellipsometer system.

$$M_{isotropic} = \begin{bmatrix} 1 & -N & 0 & 0 \\ -N & 1 & 0 & 0 \\ 0 & 0 & C & S \\ 0 & 0 & -S & C \end{bmatrix} \,. \tag{3}$$

Table 1 Detected signal intensity $I(t)$ for the most common modern ellipsometer configurations.

Rotating Polarizer/Analyzer Ellipsometer (RAE or RPE) [8]
$I(t) \propto 1 - N\cos(2\omega t) + C\sin(2\omega t)$, ω ≡ rotation frequency
(for fixed polarizer element set to 45°)
Rotating Compensator Ellipsometer (RCE) [9]
$I(t) \propto 1 + \frac{C}{2} - S\cos(2\omega t) - \frac{C}{2}\cos(4\omega t) - \frac{N}{2}\sin(4\omega t)$
(for polarizer and analyzer set to 45°, and retardance = 90°)
Phase Modulator Ellipsometer (PME) [10]
$R_\omega \propto S$, $R_{2\omega} \propto N$ (M – P = 45°, M = 45°, A = –45°)
$R_\omega \propto S$, $R_{2\omega} \propto C$ (M – P = 45°, M = 0°, A = –45°)
• R_ω and $R_{2\omega}$ are the measured intensities at the fundamental and 2nd harmonics
• M, P, and A are the Modulator, Polarizer, and Analyzer azimuthal angles (modulator amplitude = 2.405 radians)

The ellipsometric accuracy metric **E** is defined in terms of the N, C, and S parameters according to equation (8), in which N_i, C_i, and S_i are the experimentally measured values for the i'th measurement, and the primed quantities are the ideal values. **E** is root mean squared (RMS) difference over all n measurements. For ellipsometer configurations which are not sensitive to all 3 N, C, and S values, only the measurable quantities are included in the accuracy metric **E**:

$$\mathbf{E} = \sqrt{\frac{1}{3n}\sum_{i=1}^{n}\left[(N_i - N_i')^2 + (C_i - C_i')^2 + (S_i - S_i')^2\right]} \,. \tag{8}$$

RMS accuracy metrics can also be defined for other types of ellipsometric measurements. For example, ellipsometers that can directly measure N, C, and S (as opposed to calculating them from Ψ and Δ) can quantify the degree of polarization p as defined in equation (9) [3]. Since all the samples measured in this procedure are assumed strictly non-depolarizing, $p_i' \equiv 1$, the polarization accuracy metric $\mathbf{E_p}$ can be defined by (9):

$$p_i = \sqrt{N_i^2 + C_i^2 + S_i^2} \ , \quad \mathbf{E_p} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left[(p_i - 1)^2\right]} \ . \qquad (9)$$

The accuracy metric for Mueller matrix (MM) measurements $\mathbf{E_{MM}}$ is given by equation (10) (for normalized MM measurements, the '16' should be replaced by '15', as $m_{11}\equiv 1$). Equation (10) can also be used to quantify the accuracy of generalized ellipsometry (GE) measurements: the measured and ideal generalized ellipsometry data is first converted to Mueller-Jones matrices using the procedure given in [3], and then equation (10) is used to calculate $\mathbf{E_{GE}} = \mathbf{E_{MM}}$.

$$\mathbf{E_{MM}} = \sqrt{\frac{1}{16n}\sum_{i=1}^{n}\sum_{j=1}^{4}\sum_{k=1}^{4}\left[\left(m_{j,k_i} - m'_{j,k_i}\right)^2\right]} \ . \qquad (10)$$

3 Bulk sample accuracy reference The basic premise of the proposed procedure for quantifying ellipsometric accuracy is that the pseudo-dielectric function $\langle\varepsilon\rangle = \langle\varepsilon_1\rangle + i\,\langle\varepsilon_2\rangle$ of a bulk sample [5], is independent of the angle of incidence. Of course, quantifying ellipsometric accuracy by measuring and comparing $\langle\varepsilon\rangle$ vs. angle is not prudent, as the sensitivity to $\langle\varepsilon\rangle$ depends strongly on the angle of incidence.

A better approach is to calculate the ideal values for N', C', and S' in terms of $\langle\varepsilon\rangle$ (using standard Fresnel/Abeles calculations [5]), and adjust $\langle\varepsilon_1\rangle$ and $\langle\varepsilon_2\rangle$ to best fit the measured data vs. angle of incidence (which is essentially a standard ellipsometric data analysis, using a simple bulk model [5]). The figure in the abstract shows representative *N*, *C*, and *S* curves vs. angle of incidence for $\langle\varepsilon\rangle = -0.44 + 6.91\,i$ (the reference dielectric value of gold at 300 nm). Note that a wide range of *N*, *C*, and *S* values are covered over this angle range (the assumption of a bulk sample limits the accessible ranges for N and S from 0 to 1, though the entire −1 to +1 range is accessible for C). It is possible that systematic instrumentation errors could be correlated with the $\langle\varepsilon_1\rangle$ and $\langle\varepsilon_2\rangle$ fitting parameters (and thereby artificially suppressed from the accuracy metric), but quantifying this effect requires a known or assumed functional form for the systematic errors.

Two potential non-idealities, surface overlayers and angle offset, could conceivably influence the accuracy metric. However, they are easily incorporated in this scheme by simply fitting for them along with $\langle\varepsilon_1\rangle$ and $\langle\varepsilon_2\rangle$. Since these 2 parameters can be defined as common for all the wavelengths and angles, they should not introduce significant correlation into the analysis.

The bulk sample accuracy procedure described here is also applicable to generalized ellipsometry and Mueller matrix measurements: the 'isotropic' ratios/elements can be calculated from $\langle\varepsilon\rangle$, and the 'off-diagonal' ratios/elements should be zero. To probe the accuracy in the 'off-diagonal' ratios/elements, the following trick is suggested: azimuthally rotate the ellipsometer source and/or receiver optics, and acquire data vs. angle of incidence (without recalibrating). This induces numerous features in the 'off-diagonal' ratios/elements, all of which are simply parameterized by $\langle\varepsilon_1\rangle$ and $\langle\varepsilon_2\rangle$ at each wavelength, and 2 coordinate rotation values which are common to all wavelengths and angles.

4 Experiment The ellipsometric accuracy of a prototype dual rotating compensator ellipsometer system [4] was characterized using the previously described method. Data were acquired at >1000 wavelengths over a 245–1000nm spectral range, and 21 angles of incidence from 30–80°, in the straight-through and off the 3 bulk-like reference samples: a silicon wafer with native oxide (Si), an optically thick gold film on glass (Au), and a ½" thick fused silica optical flat (Fused Silica).

Table 2 shows the ellipsometric accuracy metrics that were determined from the data. Note that most values are significantly less than 0.001, which corresponds to better than 0.05% accuracy (as the MM elements are bound from −1 to +1). Adding surface overlayers and angle offset to the analysis only slightly improves the accuracy metrics, this validates the bulk substrate assumption and confirms the angle of incidence accuracy.

Relative to the immense amount of data acquired, only a few representative subsets are plotted in Figures 1–5. Figures 2 and 3 illustrate the wide range of N, C, S and MM element values which are accessible by the measurements. In these figures, only the measured data are shown, as the ideal data curves would be indistinguishable on this scale.

Representative spectroscopic difference plots are shown in Fig. 4. While a few angles exhibit systematic offsets, and increased noise is visible in certain spectral ranges, most data are within ±0.001 of the ideal values. Figure 5 shows a difference plot of the 15 normalized Mueller matrix elements vs. angle, acquired on the Au

Table 2 Ellipsometric accuracy metrics (over 245–1700 nm, 30 – 80°) for a prototype dual rotating compensator ellipsometer.

	Sample	**E**	$\mathbf{E_p}$	$\mathbf{E_{GE}}$	$\mathbf{E_{MM}}$
Straight-Through		0.00034	0.00049	0.00049	0.00064
	w/optics rotated	–	–	0.00057	0.00083
Si	Ideal Bulk	0.00049	0.00158	0.00050	0.00091
	w/Oxide	0.00048	0.00158	0.00050	0.00091
	w/Oxide +ϕ_{offset}	0.00039	0.00158	0.00047	0.00088
	w/optics rotated	–	–	0.00049	0.00084
Au	Ideal Bulk	0.00046	0.00162	0.00059	0.00121
	w/Roughness	0.00042	0.00162	0.00058	0.00120
	w/Roughness +ϕ_{offset}	0.00038	0.00162	0.00056	0.00119
	w/optics rotated	–	–	0.00056	0.00090
Fused Silica	Ideal Bulk	0.00071	0.00187	0.00083	0.00171
	w/Roughness	0.00070	0.00187	0.00083	0.00171
	w/Roughness +ϕ_{offset}	0.00064	0.00187	0.00081	0.00169

sample. Only 4 fit parameters (⟨ε_1⟩, ⟨ε_2⟩, and the azimuthal rotation angles of the source and receiver optics) were required to fit all 15 MM curves in Fig. 3 to the level of accuracy shown in Fig. 5.

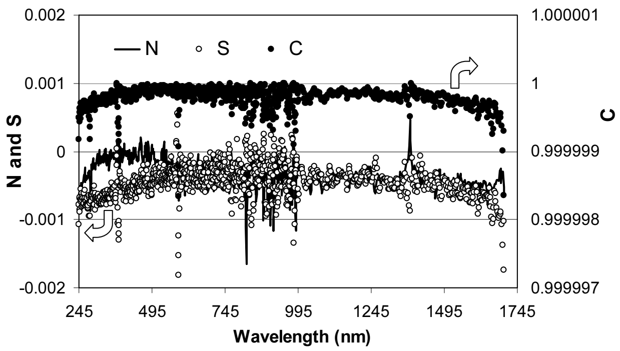


Figure 1 Straight-through ellipsometric data.

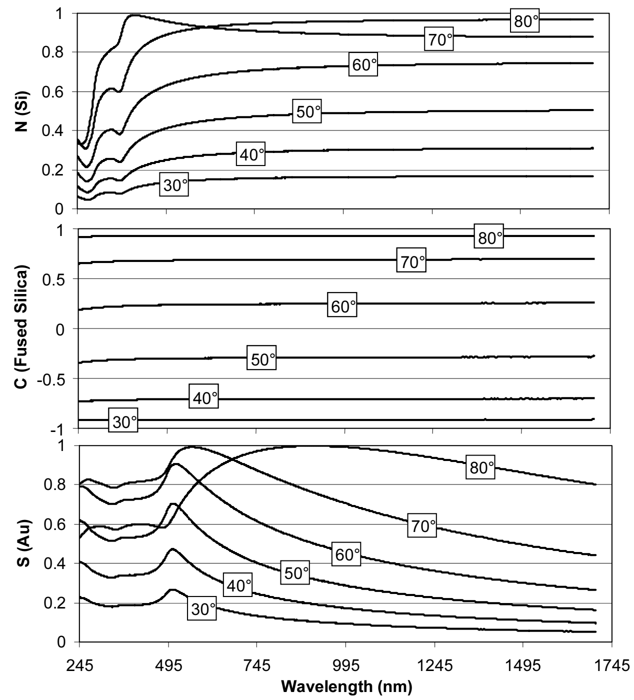


Figure 2 Subsets of the measured *N*, *C*, and *S* data acquired from the 3 reference samples, plotted at selected angles.

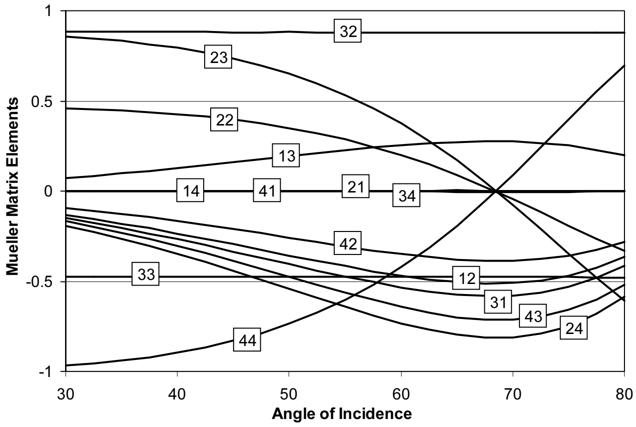


Figure 3 Mueller Matrix (MM) data vs. angle acquired on Au with rotated optics (source = +45°, receiver = +15°), at 300 nm.

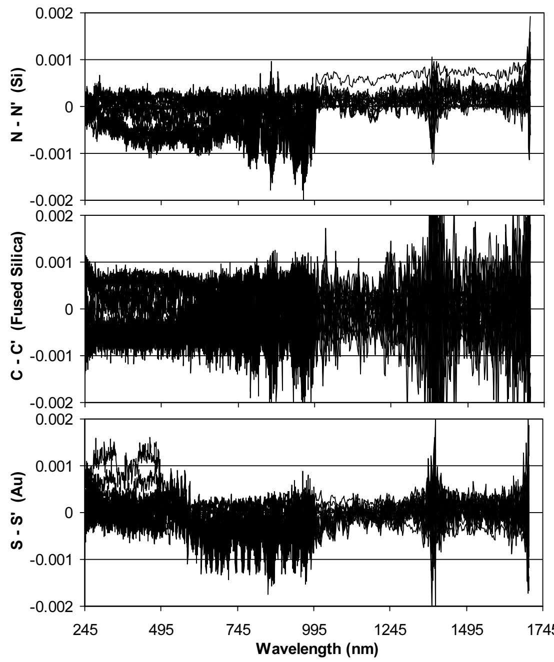


Figure 4 Difference between measured and ideal *N*, *C*, and *S* for the 3 reference samples, plotted for all measured angles 30 – 80°.

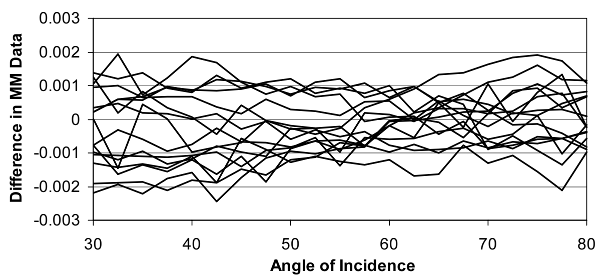


Figure 5 Difference between the measured MM data shown in Fig. 3 and the ideal data calculated from the bulk model.

5 Conclusion The proposed method quantifies the ellipsometric accuracy over a wide range of ellipsometric values, using readily available reference samples. The main drawback of the method is the requirement of variable angle of incidence data. The accuracy of a dual rotating compensator ellipsometer system characterized by this method significantly exceeds a 0.1% accuracy target.

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